| X-ray Absorption Near Edge Structure of Amino Acids and Peptides | X1A |
|---|---|

J. Boese, A .Osanna, C. Jacobsen, J. Kirz, E. Tall (SUNY Stony Brook), and X. Zhang (Harvard U.)

Combination of the spatial resolution of soft x-ray microscopes with x-ray absorption near-edge structure (XANES) analysis provides a new means for chemical state mapping [1]. Comparison of near edge absorption resonances with reference spectra makes it possible to map the concentrations of different double bonds. We tried to explore the applicability of this method to protein specific imaging. All proteins in living systems consist of only 20 different amino acids, linked together via the peptide bond. We wanted to find out if a protein spectrum can be predicted from amino acid spectra. This depends on how much spectra are affected by the peptide bond.

Preliminary work by X.Zhang and S.Williams [2] showed that a nitrogen edge XANES spectrum of the dipeptide consisting of arginine and aspartic acid was just the sum of the spectra of the two monomers. We have measured carbon edge XANES spectra of amino acids for the first time. Spectra of six amino acid monomers, four dipetides and one tripeptide were compared. Because of their heat sensitivity, amino acids cannot be evaporated but have to be analyzed in solid form. In order to obtain quantitative absorption measurements using transmission spectroscopy, the illuminated spot of the sample has to be of uniform thickness. Therefore a special sample preparation technique was used, and the spectra were obtained using the small spot size of the Stony Brook scanning transmission x-ray microscope at beamline X1A.

The spectra of the dipeptides and tripeptides investigated can indeed be explained as the sum of the spectra of the monomers involved. A typical result is presented in Figure 1. The spectra of glycine (Gly), tyrosine (Tyr), and the Gly-Tyr dipeptide (solid lines) are shown together with a weighted sum of the two monomer spectra (dashed line). The peptide bond has only a very small effect on spectra analyzed. It causes a very small shift ($\approx$0.3 eV) of the $\pi^*$ resonance near 289 eV towards lower energies. If this result holds in general, it would allow the prediction of spectra of simple proteins, which could be used in protein specific imaging with x-ray microscopes.

[1] X.Zhang, R.Balhorn, J.Mazrimas, J.Kirz *J.Struct.Biol.*,116:335-344,1996
[2] X.Zhang Ph.D. Thesis, SUNY at Stony Brook, May 1995

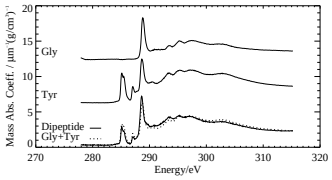


Figure 1.